Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Enhanced performance of Mo_2P monolayer as lithium-ion battery anode materials by carbon and nitrogen doping: a first principles study

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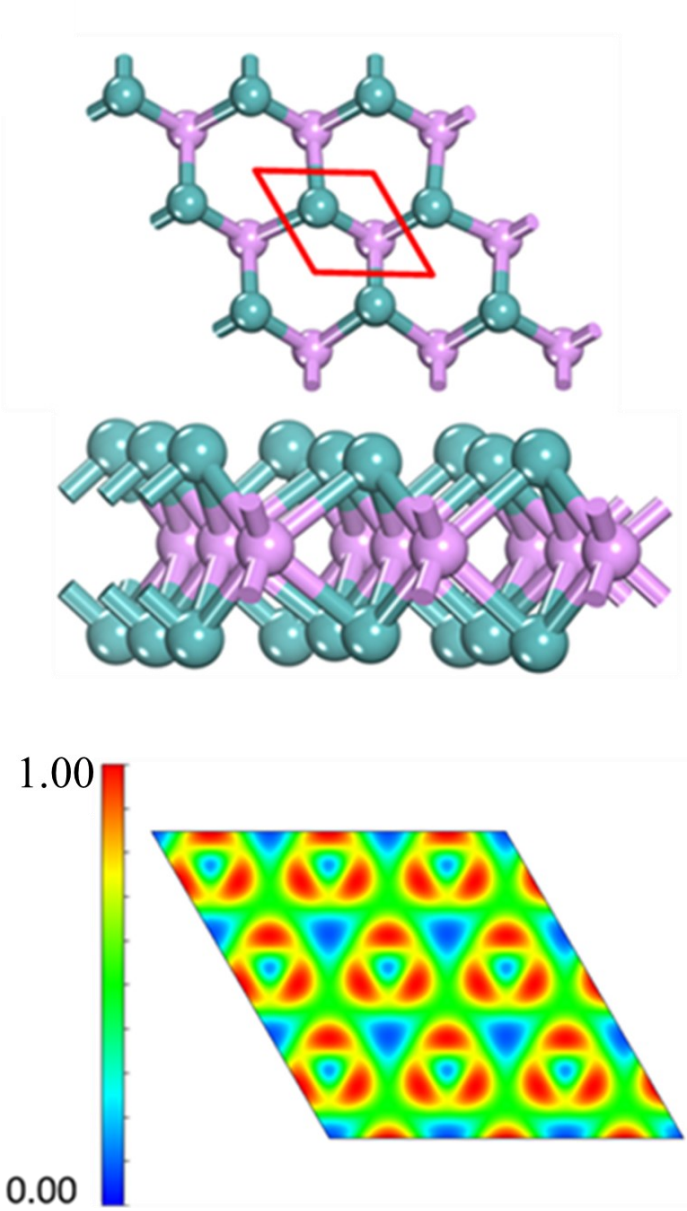


Fig. S1 Top and side views of the optimized structure of Mo_2P monolayer, and its contour plots of the electron localization function (ELF). The pink and blue balls represent P and Mo atoms, respectively. The red line outlines a (1×1) surface unit cell.

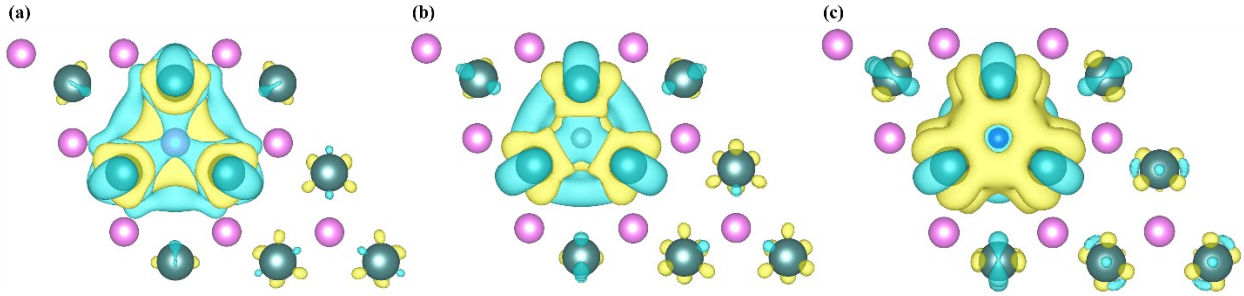


Fig. S2 The charge density difference of (a) Mo_2P, (b) CMP, and (c) NMP. The yellow and cyan regions represent electron accumulation and depletion. The pink, blue, grey, and dark-blue balls represent the P, Mo, C, and N atoms. The isosurface value is 0.0015e/bohr^3.

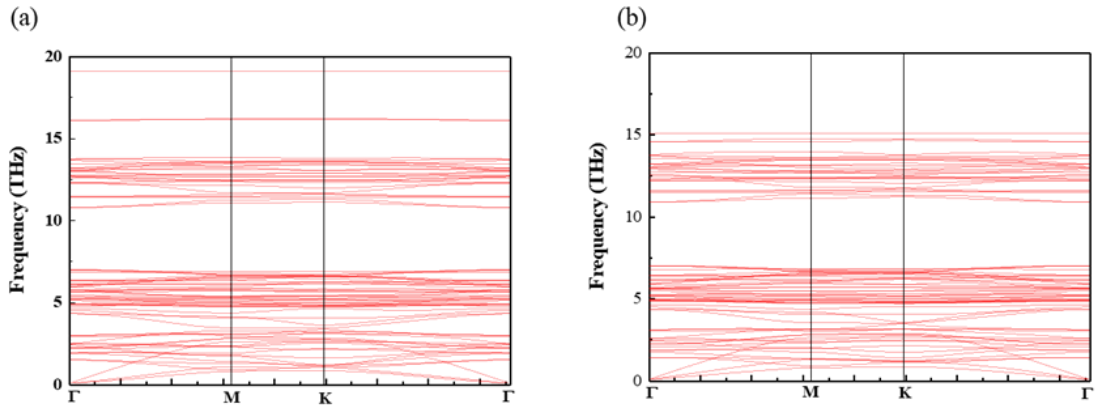


Fig. S3 Phonon dispersions of the free-standing (a) CMP and (b) NMP monolayers. The absence of any imaginary modes confirms their dynamic stability.

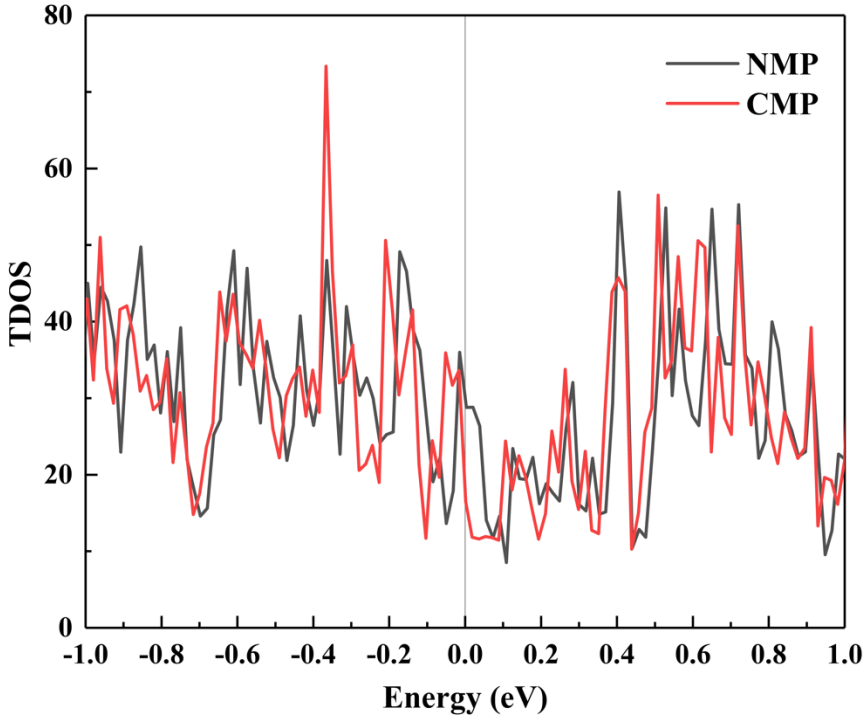


Fig. S4 The total density of states (TDOS) of the free-standing CMP and NMP monolayers. The Fermi level is set at zero energy.

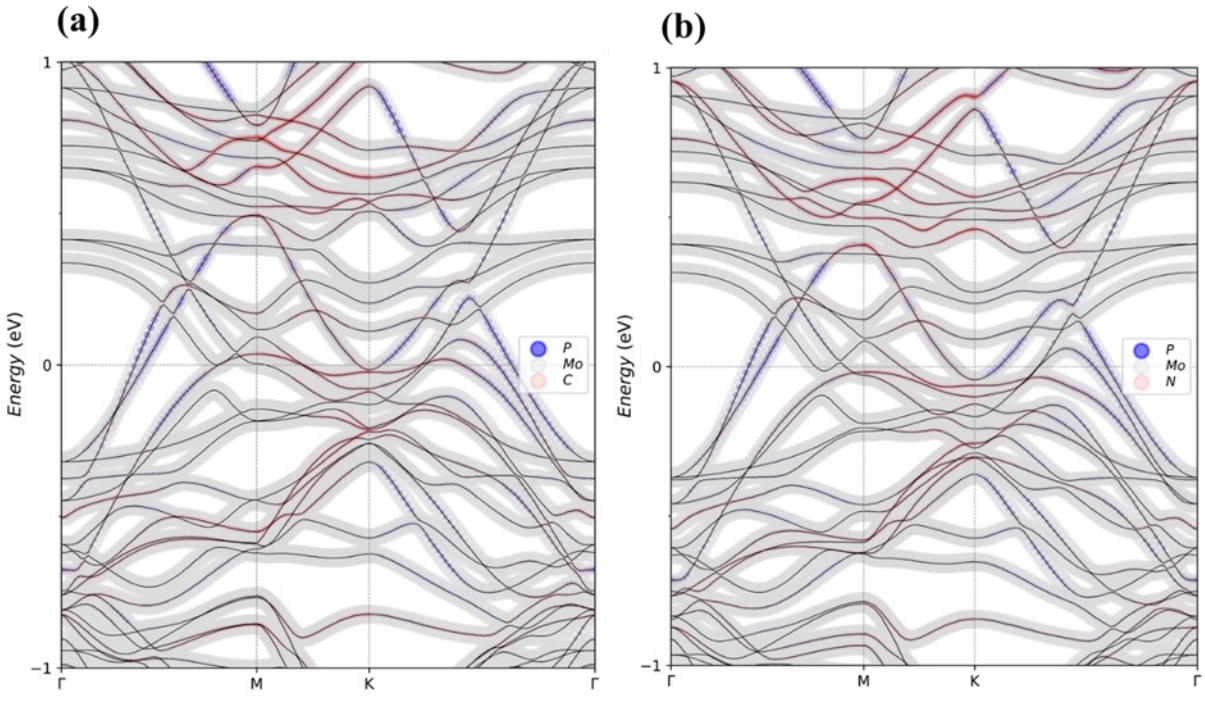


Fig. S5 The projected band structure in (a) CMP and (b) NMP monolayers. The blue, grey and red curves denote P, Mo, and C(N) sum of orbits, respectively, and the thickness represents the weight of each atom orbitals. The Fermi level is set at 0 eV.

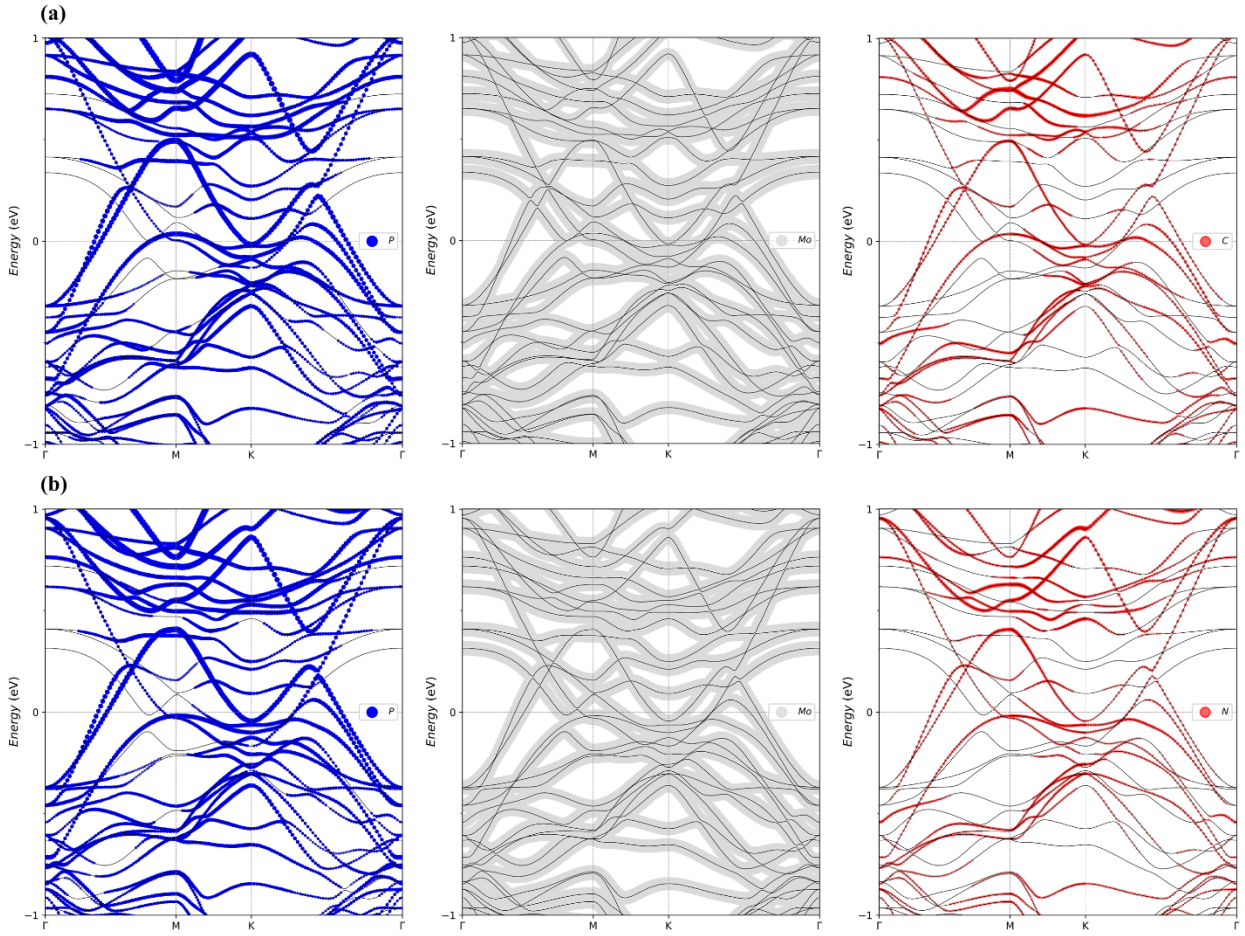


Fig. S6 The projected band structure of each atom for in (a) CMP and (b) NMP monolayers. The blue, grey and red curves denote P, Mo, and C(N) sum of orbits, respectively, and the thickness represent the weight of each atom orbitals. The Fermi level is set at 0 eV.

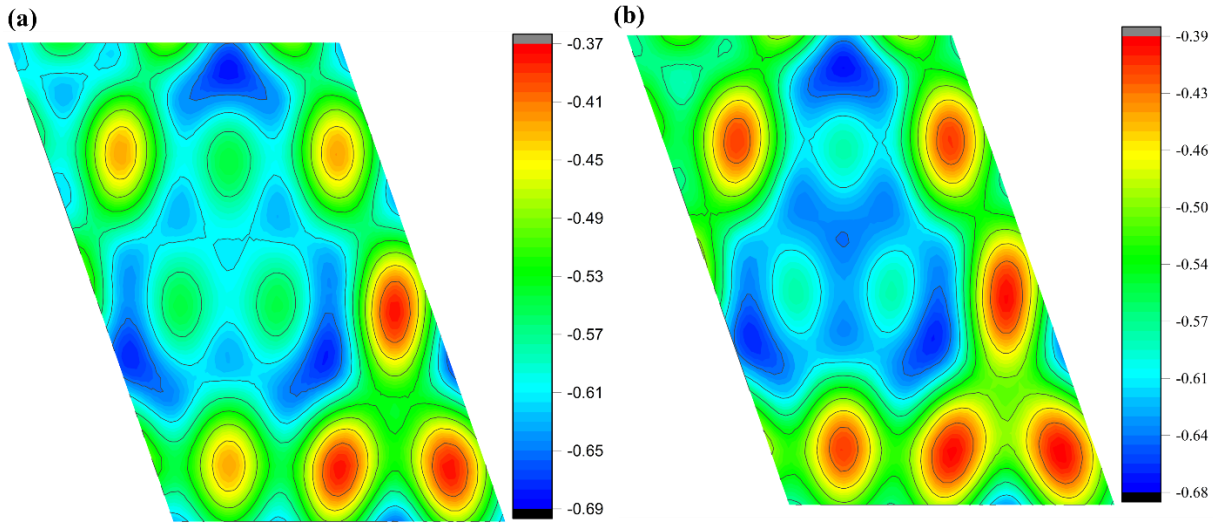


Fig. S7 The potential energy surfaces of a Li adatom (a) on CMP and (b) on NMP monolayers. The contour spacing in (a) 0.04 eV while it is 0.03 eV in (b).

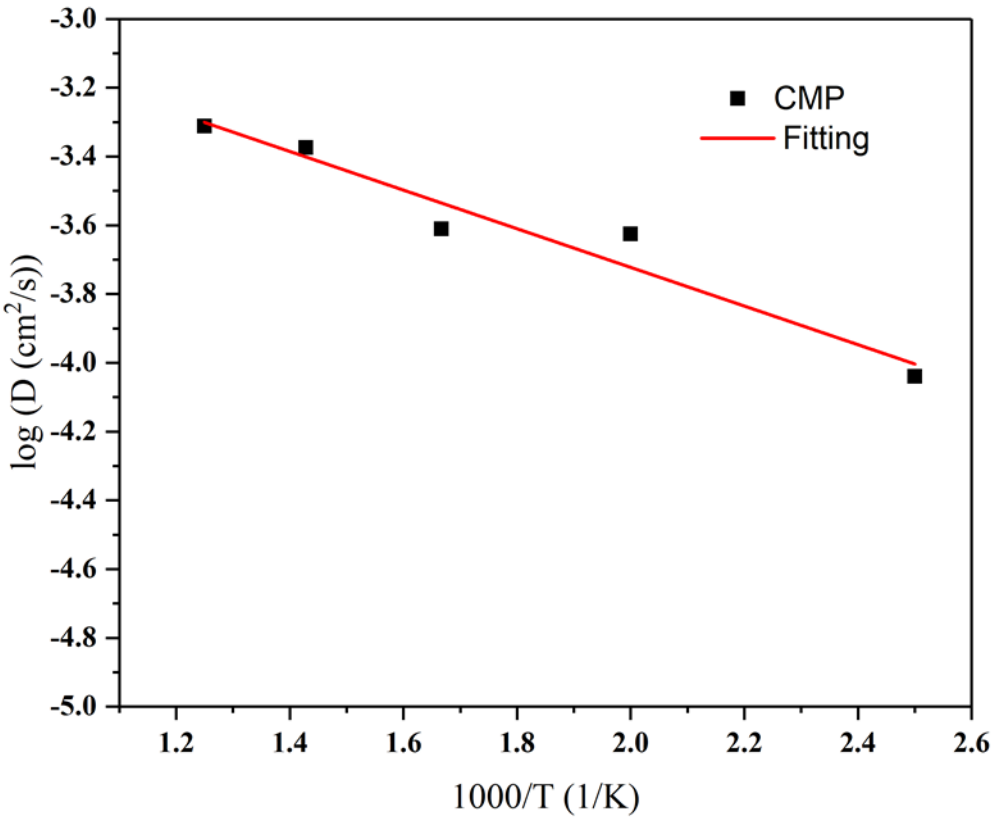
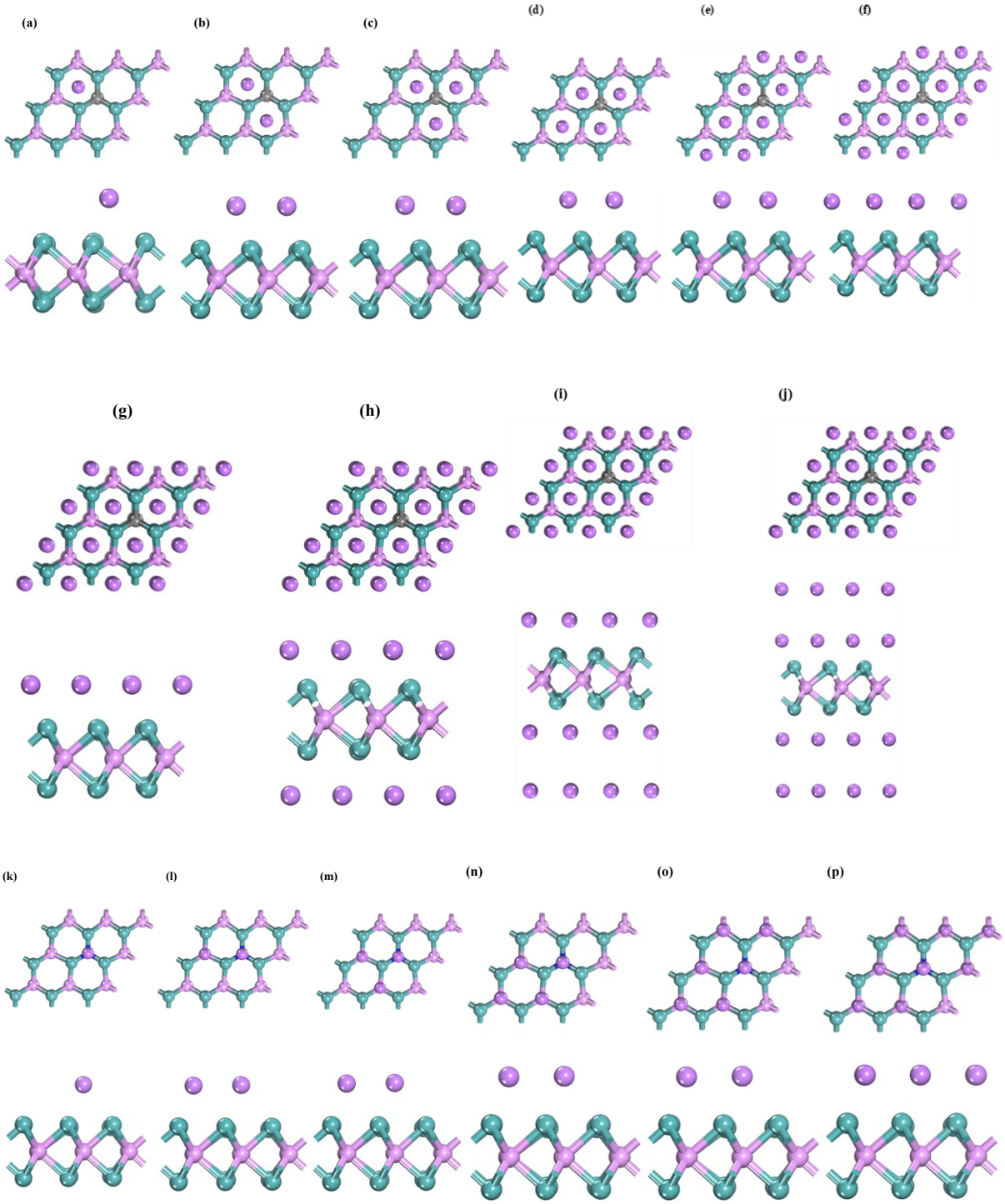


Fig. S8 Arrhenius plot of CMP overall diffusion coefficient and the fitting line.


(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
(j)
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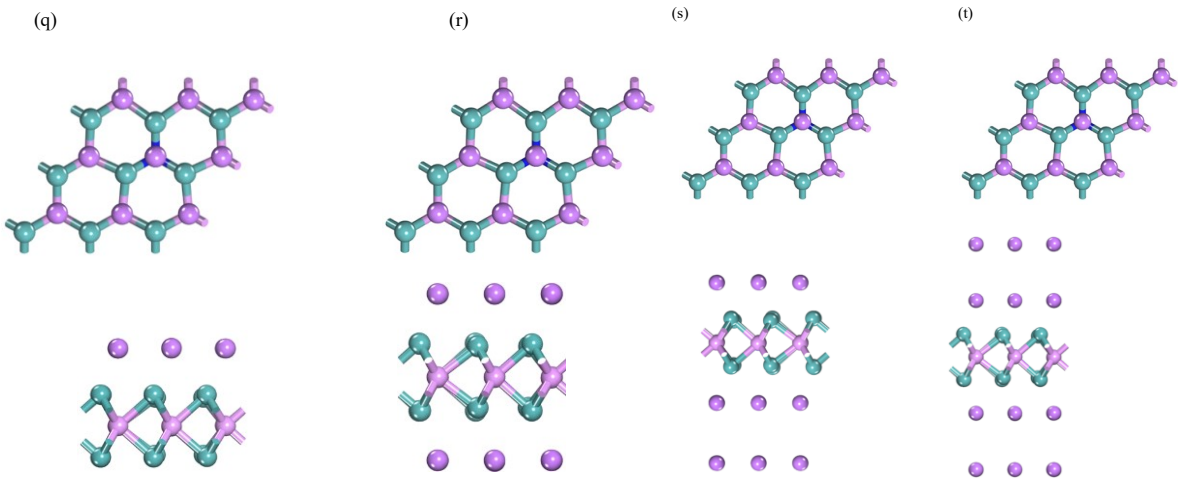

Fig. S9 (a)-(j) Top and side views of monolayer CMP with different coverage of Li atoms for $Li_{0.028}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.056}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.083}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.111}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.167}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.222}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.25}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.5}Mo_{0.50}P_{0.222}C_{0.028}$, $Li_{0.75}Mo_{0.50}P_{0.222}C_{0.028}$, and $Li_{1}Mo_{0.50}P_{0.222}C_{0.028}$, respectively. (k)-(t) Top side views of monolayer CMP with different coverage of Li atoms for $Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.056}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.083}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.111}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.167}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0,222}$ $Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.25}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.5}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, $Li_{0.75}Mo_{0.50}P_{0.222}N_{0.028}$, and $Li_{1}Li_{0.028}Mo_{0.50}P_{0.222}N_{0.028}$, respectively. The pink, blue, grey, and dark blue balls represent P, Mo, C, and N atoms, respectively.

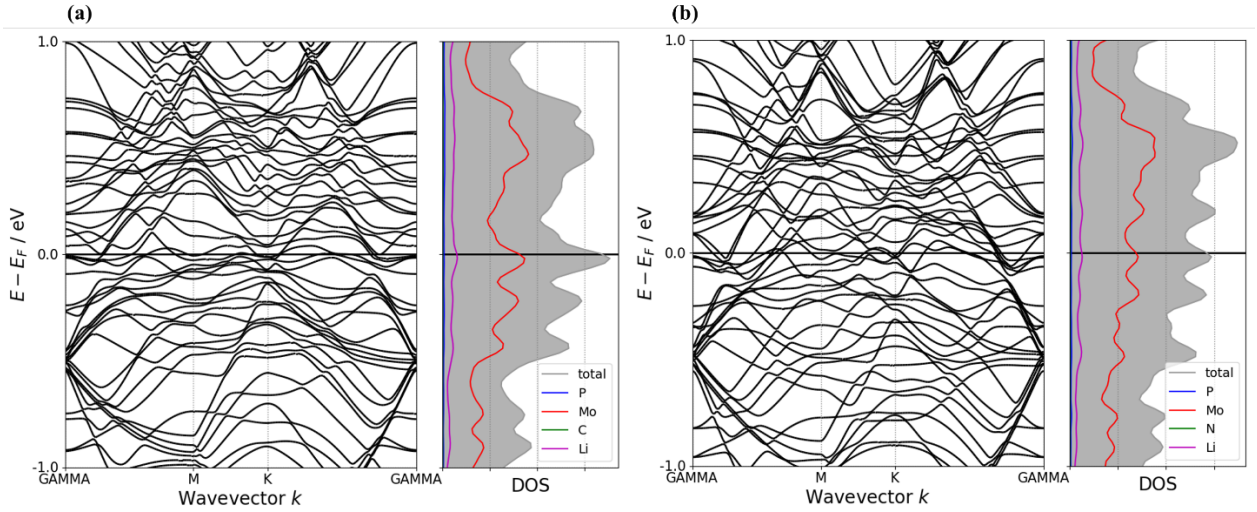

Fig. S10 The electronic band structure and projected densities of states of (a) CMP and (b) NMP monolayers at 100% lithiation states (including 36 atoms in the supercell containing 27 atoms).

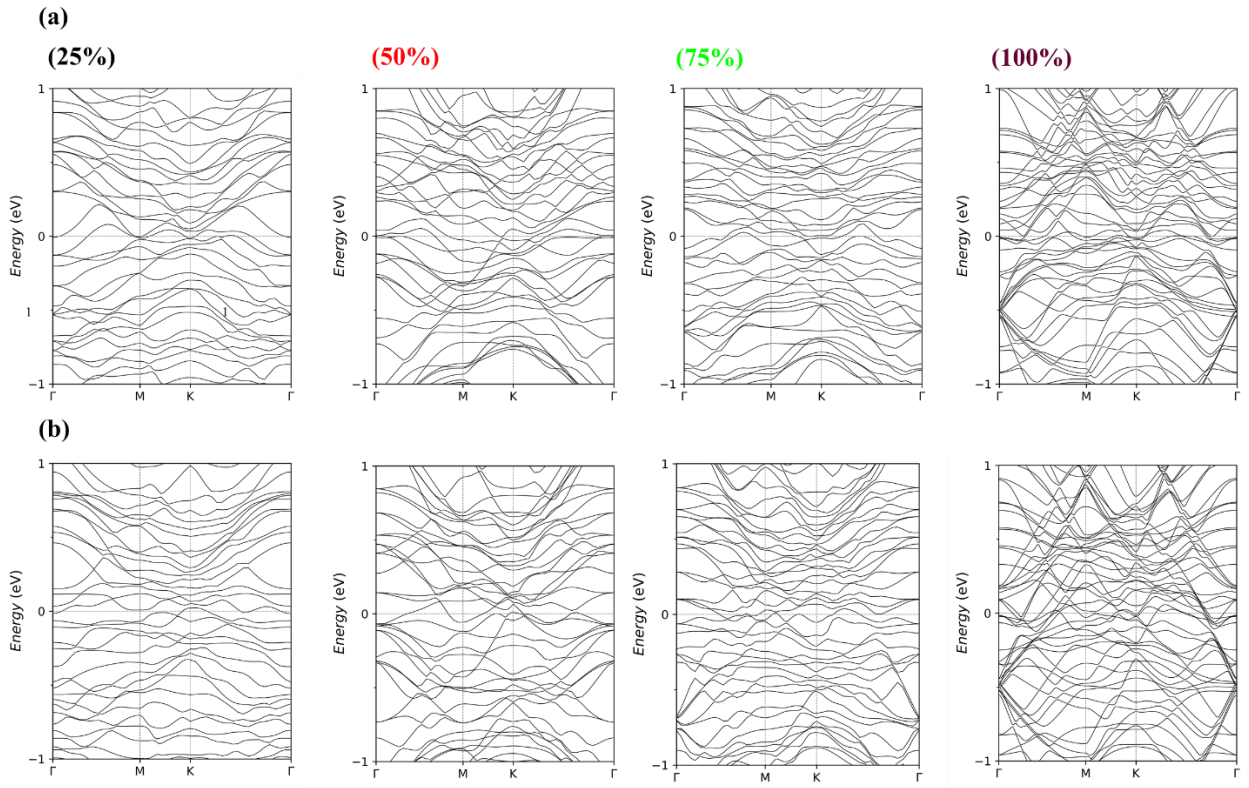

Fig. S11 The electronic band structure of (a) CMP and (b) NMP monolayers at different degree (25% ~ 100%) lithiation states.

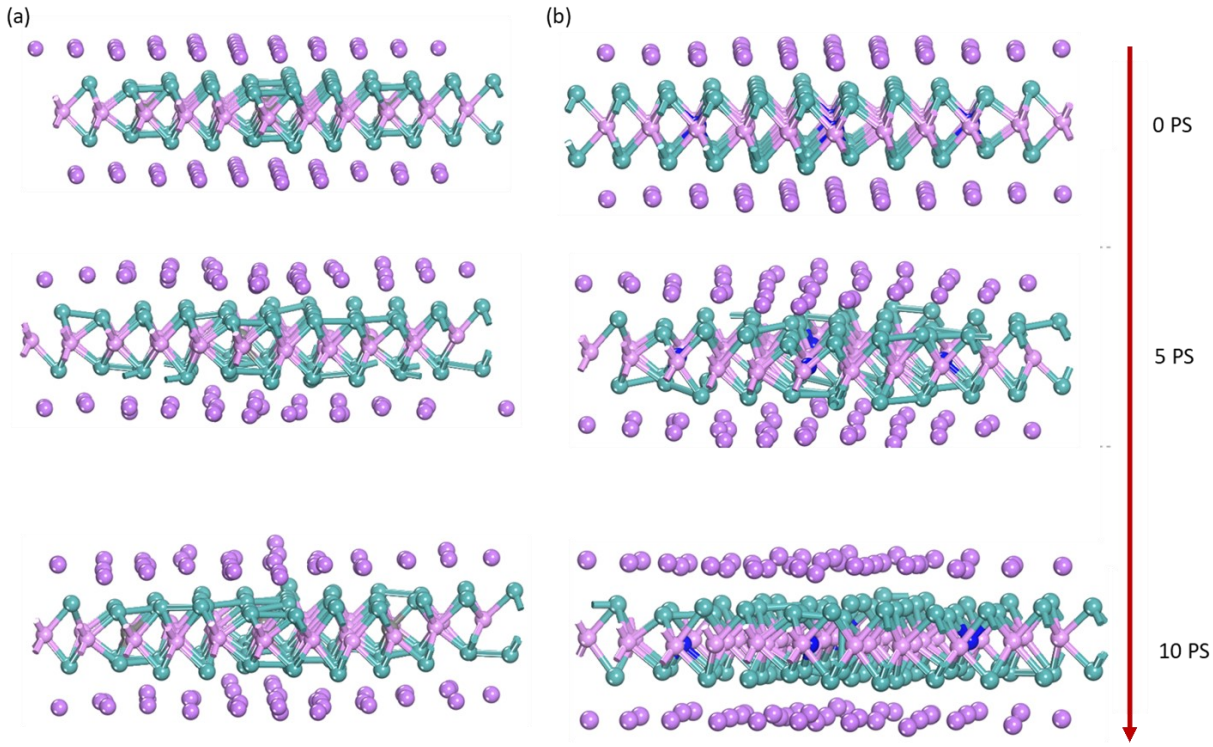

Fig. S12 (a) Snapshots of trajectories for the CMP monolayer (a) and NMP monolayer at the end of 10 ps AIMD simulations at 300 K. The pink, blue, grey, and navy balls represent P, Mo, C, and N atoms, respectively.

Table S1 Diffusion coefficient with different temperatures calculated using AIMD.

Temperature (K)	Diffusion Coefficient (cm^2/s)
400	9.12E-05
500	2.37E-04
600	2.45E-04
700	4.23E-04
800	4.88E-04